Module 4: Improving the Environmental Performance of Unit Operations and Flowsheets

David Shonnard
Department of Chemical Engineering
Michigan Technological University

Module 4: Improving the Environmental Performance of Unit Operations and Flowsheets

- Educational goals and topics covered in the module
- Potential uses of modules in chemical engineering courses
- Student handouts
- Instructor materials
- Software
- Case study / Software Demonstrations

Module 4: Educational goals

Students will:

- become aware of the mechanisms of waste generation in selected unit operations
- learn of ways to reduce waste generation for selected unit operations
- be able to apply basic input/output environmental assessment for selected unit operations

Module 4: Topics covered

- Mechanisms of waste generation for a ***Storage Tank*** and a ***Reaction Network***
- Use of OPPT Software Tools to evaluate pollution prevention efforts
- Basic environmental risk metric : input/output screening

Module 4: Potential uses of the module in chemical engineering courses

- Plant Design course:
  - » Input/output environmental screening of unit operations selection and improvement efforts
  - » Improvement of environmental performance of a flowsheet
- Reactor Design Course:
  - » Optimize reactor configuration (reactor type, temperature, residence time, mixing, etc.)
  - » Incorporate environmental considerations
- Unit Operations Course:
  - » Heat exchanger design calculations to minimize waste generation

Module 4: Student handouts

- Chapter 9 textbook outline: ***Unit Operations and Pollution Prevention***
- Class lecture notes:
  - » edited from chapter 9
  - » instructor writes in key concepts and calculations during the lecture
- Example Problems:
  - » 1. Storage Tank pollution prevention
  - » 2. Reactor Design pollution prevention

Module 4: Instructor materials

- Completed class lecture notes:
  - » edited from chapter 9
  - » contains material that the instructor writes into the notes during the lecture
- Example Problem Solutions:
- Software for estimating storage tank emissions & environmental metric properties

Module 4: Emissions estimation software

- Emissions: Tanks4 ; EPA 1999

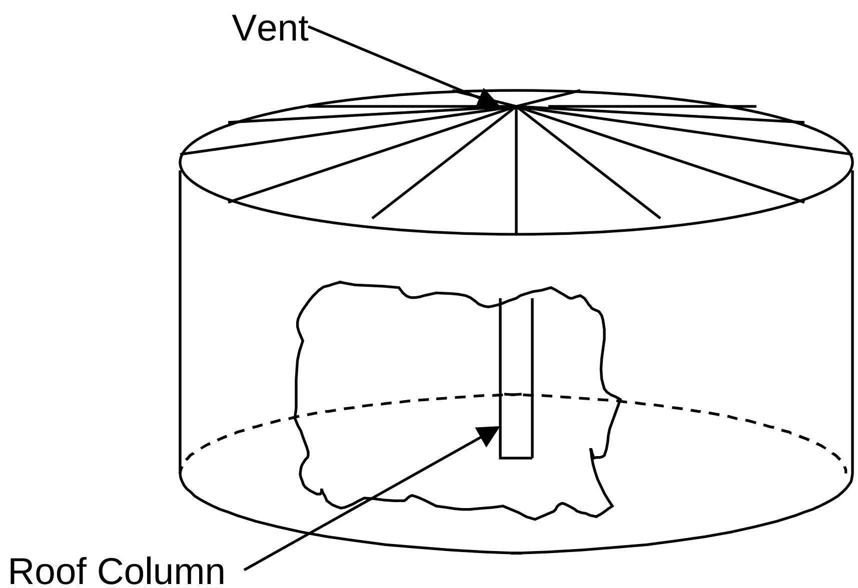
- Environmental Parameters ; OPPT Tools

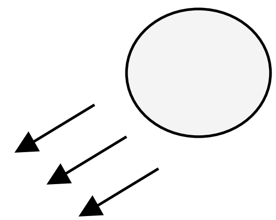
SOFTWARE DEMONSTRATION

Module 4: Storage tank pollution prevention

Emission Mechanisms; Fixed Roof Tank

$L_T = L_S + L_W$





<u>Vapor pressure of liquid drives emissions</u>

ΔT	↕	- Weather, paint color/quality
ΔP	↕	- Weather
Liquid Level	↕	- liquid throughput, volume of tank

Module 4: Example problem: reducing storage tank emissions ; Comparisons

- Type of Tank:
  - » Vertical Fixed Roof Tank
  - » Internal Floating Roof Tank
  - » Domed External Floating Roof Tank

- Tank Operation and Condition:
  - » Heated versus unheated tank
  - » White paint versus dark paint
  - » New versus poor quality paint

Module 4: Storage tank comparison

Gaseous Waste Stream Flowsheet

- Toluene emissions only
- 100 kgmole/hr absorber oil rate
- 15,228.5 gallon tank for each comparison

Storage Tank Type	Vertical Fixed Roof	Internal Floating Roof	Domed External Floating Roof
Annual Emissions (lb)			
White Paint	337.6	66.2	42.8
Grey (Medium) Paint	489.1	85.1	52.4
Heated (White)	313.5		
Poor (Grey/Medium)	509.7	81.0	51.5

Module 4: Storage tank example problems

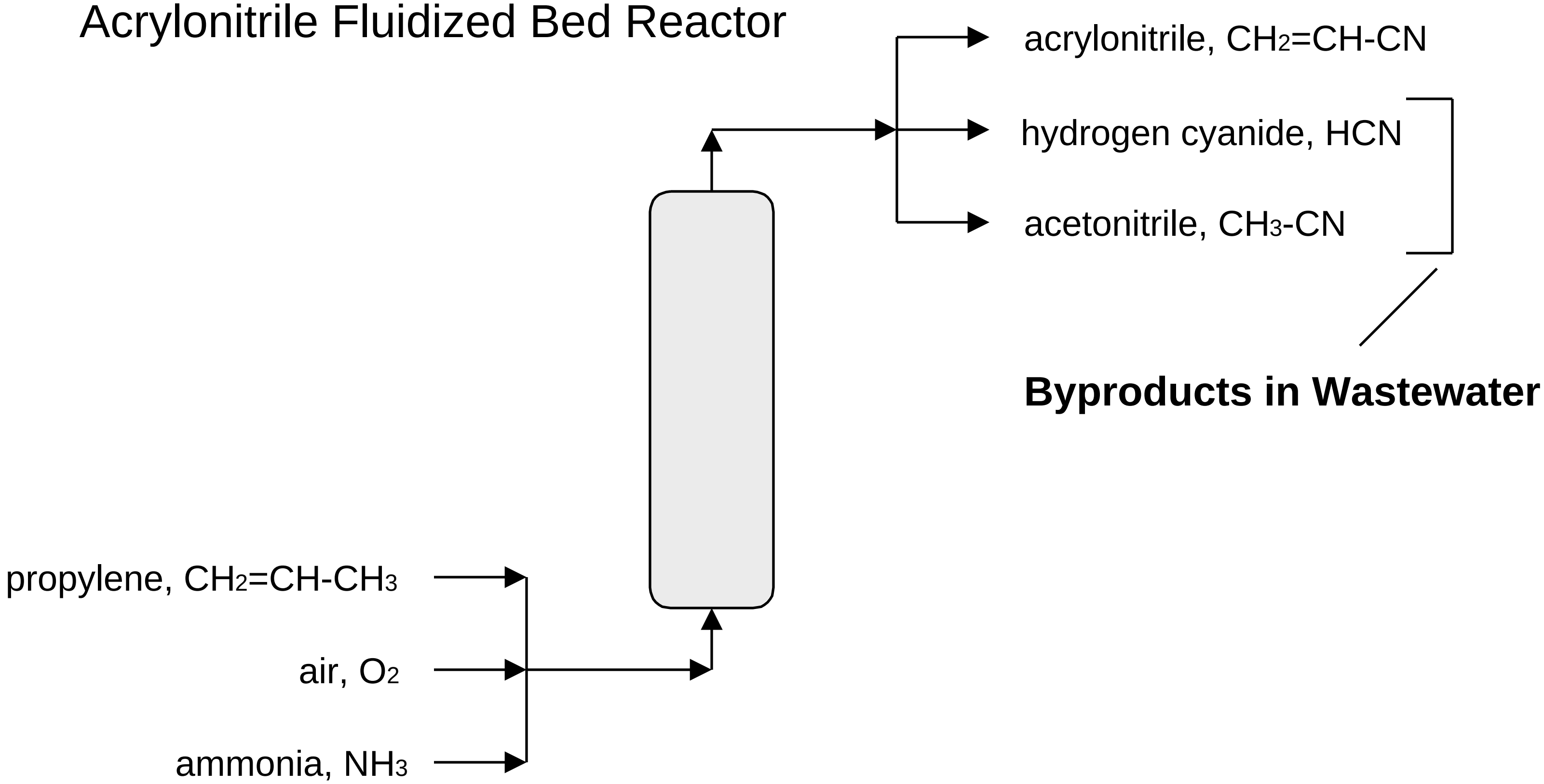
- Compare incremental costs of fixed and floating roof tanks for pollution reduction
  - » Capital (floating roof) versus operating (pollution control on fixed roof) costs
- Calculate net solvent emissions reduction for application of new paint to existing fixed roof tank
  - » Old dark paint in poor condition
  - » New white paint, 50% (vol) solvent in paint, 100 sq. ft./gal of paint

Module 4: Reactor pollution prevention

- Reactor Type
  - » CSTR versus PFR
  - » Fixed Bed versus Fluidized Bed
- Reactor Conditions
  - » Temperature
  - » Residence time
  - » Mixing
  - » Control of critical parameters
- Waste formation reactions
  - » Parallel and series reactions

Module 4, Acrylonitrile example; Optimize for reactor conditions (Hopper,et al. 1992)

Acrylonitrile Fluidized Bed Reactor



Module 4, Use of OPPT Tools to optimize reactor conditions

- Traditional Approach
  - » Optimize based on selectivity and conversion
  - » Reduce total byproduct mass generation
  - » No risk assessment
- Risk-Based Approach
  - » Incorporate screening level risk assessment
  - » Use OPPT tools to provide parameters
  - » Convert byproduct generation from mass basis to risk basis

Module 4, Risk Index (EPAs WMPT)

Risk = Toxicity x Exposure

Toxicity = Reference Dose (RfD) (ingestion)

EPA TTN Web (http://www.epa.gov/ttn/uatw/hlthef/)

Exposure = ***F*** x ***Mass*** x ***Persistence*** x ***Bioaccumlation***

F = fraction of byproduct removed in wastewater treatment

EPA OPT Tool (EPIWIN)

Mass = mass rate of waste generation in reactor

Predicted by reactor model

Persistence = Biodegradation Timeframe

EPA OPPT Tool (BIOWIN)

Bioaccumulation = Bioconcentration Factor (BCF)

EPA OPPT Tool (BCF)

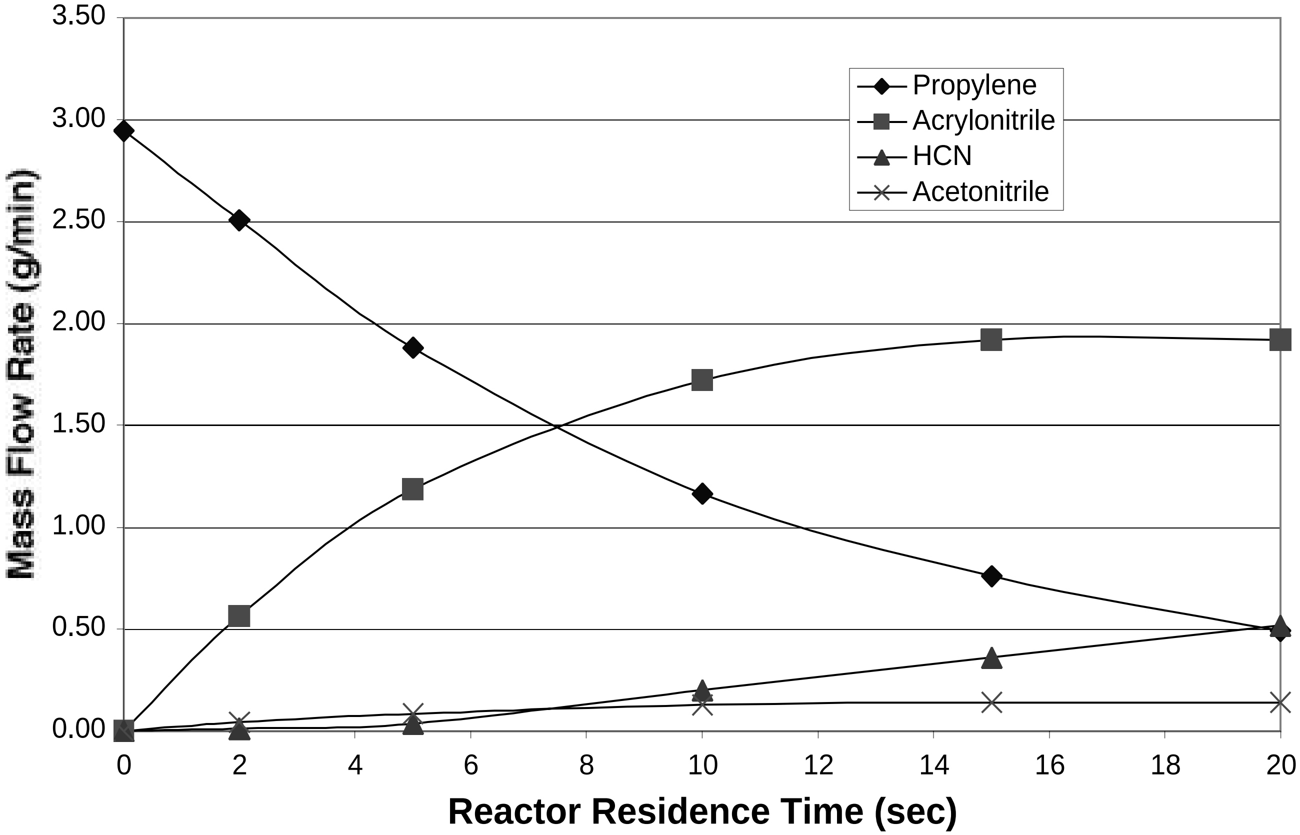
Module 4, Risk profiles of byproducts

Acetonitrile has a greater risk potential due to higher toxicity and lower removal percentage in wastewater treatment

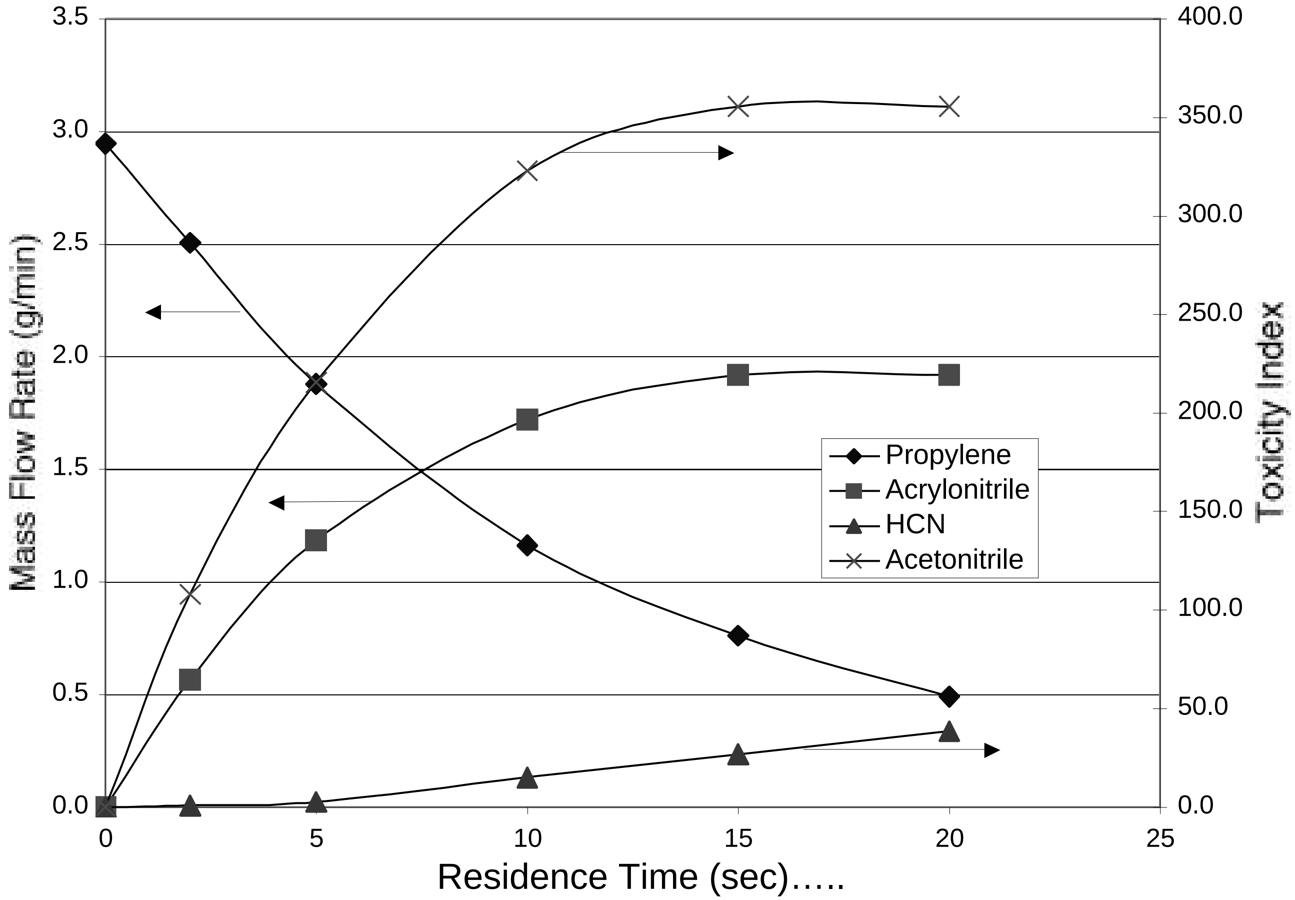
Chemicals	Removal Efficiency (%)	Toxicity, Reference Dose (mg/kg/d)	Persistence, Biodegradation Timeframe (d)	Bioaccumulation, (BCF)
HCN	90.51*	0.02	5	3.16
Acetonitrile	3.67	0.006	5	3.16

* Volatilization to Air in wastewater treatment plant

Module 4, Reactor residence time results
Mass Basis; 400˚C



Module 4, Reactor residence time results; Risk Basis ; 400˚C



Module 4, Reactor residence time; Conclusions

- Traditional mass-based optimization
  - » Choose reactor residence time to minimizing total mass waste generation (HCN + CH_2O=CN)
- Risk-based optimization
  - » Choose reactor residence time to minimizing total risk generation (HCN + CH_2O=CN)
- Focus on minimizing CH_2O=CN over HCN
  - » Changes optimization target

Module 4: Summary of Software Needed

1. COMMERCIAL PROCESS SIMULATOR
   » mass balances, energy balances, stream data, equipment sizes, air/water releases
2. UNIT OPERATION MODELS
3. AIR EMISSIONS ESTIMATION
4. Environmental/Toxicological Properties Estimator (EPIWIN, ONCOLOGIC)